Creation of Sodium Crystal Modifications by Molecular-Dynamics Modeling

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Crystallization of supercooled sodium with the formation of its different modifications was studied by a molecular-dynamics method. The FCC sodium crystal has been produced as a result of creating a 43-atomic embryo in a system of 500 particles while the growth of the BCC crystal has been initiated by a 51-atomic one when the system contained 686 particles. The internal energy of the BCC crystal is lower than that of the FCC crystal at the same density and temperature. The value of the energetic barrier between the two crystal modifications is more than two times less than that between the BCC crystal and the supercooled liquid. Topological differences of BCC and FCC packings are explained by the special construction of Wigner-Seitz cells of the BCC and FCC lattice.

We have also investigated the crystal growth when the initial crystal fragment was presented by a combination of BCC and FCC lattices. The result of the crystallization depended on the fragment size. At first the 43-atomic embryo (21-BCC,1-FCC and 1 common atom) was reconstructed to the destroyed BCC structure with the internal energy decreasing by ~1%. Then crystallization to the BCC lattice took place at a change in energy more than by 10%. A complicated process of crystallization was observed when the size of the initial combination embryo was 80 atoms (40-BCC and 40-FCC). At first the intermediate boundary between the BCC and FCC parts of the embryo was formed at a slow decrease of the internal energy by ~4%. Then crystallization took place decreasing sharply the energy of the system yet by another ~2.4%. Moreover the BCC lattice appeared at one side of the boundary and the FCC - at the other one that one can see from the construction of Voronoi polyhedra and projects of particle coordinates.